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SOLID PROPELLANT COMBUSTION
MECHANISM RESEARCH

1977-1978 Annual Report

Prepared by

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1.0 TECHNICAL OBJECTIVES

This annual report summarizes the progress which is being made on the research on steady combustion processes of nitramine monopropellants and on the effects of extended flame zones on rocket motor flow and pressure responses. Attention is being focused on nitramines (e.g., HMX and RDX) ingredients which are prominent in the Navy's plans for improved rocket propellants.

Until now, investigations of items such as unsteady chamber flow, flame structure, chemical kinetics, and mechanistic chemical interaction have been conducted largely independently of each other. There is a continuing need for the investigators working in the various disciplines to interact and to give more attention to applying the results of research evolving from their areas of specialization. The mathematical models which are being developed and refined as part of the study provide many opportunities to use the measurements and theories of other investigators. As part of this study, our efforts are being closely coupled with investigations being conducted in other laboratories. This is being accomplished as we acquire data for use in the models, incorporate into the models the chemical mechanisms proposed by others, and critique the calculated results in terms of the input data and chemical mechanisms.

2.0 STATUS OF CURRENT RESEARCH

Two portions of our research will be summarized briefly in this section. For more details, the readers are referred to the complete papers abstracted in Section 3.0.

2.1 Unsteady Reacting Flows in Solid Rocket Chambers

The unsteady responses of flowing, high-temperature gases in solid propellant rocket chambers are usually analyzed by assuming a thin or collapsed chemical reaction zone, adjacent to the solid propellant surface. This assumption implies that the characteristic relaxation times for condensed phase, surface reactions, and gaseous flame zone are $\tau_c > \tau_s \gg \tau_g$. Thus, for moderate frequencies, the thermal relaxation time in the condensed phase would be rate determining, while the gas phase and surface reaction processes may be considered quasi-steady, in the sense that they adjust to any change of parameters much faster than the condensed phase. When the surface of the chamber control volume is taken at the outer edge of the fully reacted flame, the propellant and flame may thus be considered a nonsteady mass source in the overall chamber-propellant configuration, whereas the fully reacted chamber gases act as a wave-carrying medium.

Clearly, the quasi-steady gaseous flame zone assumption holds for a large class of solid propellants whose characteristic chemical relaxation time in the gas phase is sufficiently short. However, that assumption does not apply for several important types of propellants which exhibit relatively long secondary reaction zones, e.g., nitrocellulose-based and some nitramine composite propellants.^{1*} A more precise qualitative idea of what is meant by "long" chemical reaction zones is given by the following interactions between the pertinent physical length and time scales.

- (a) The comparison of a local characteristic reactive length scale, δ_R (using mean reaction rate near the propellant surface) with a fluid dynamic dimension such as the

*References for this section are given in Section 2.1.4.

boundary layer displacement thickness, δ_{disp} , can indicate the extent of chemical reactions in the main chamber flow (for an internally burning grain):

$$\delta_R / \delta_{\text{disp}} \sim O(1) \quad (1)$$

or larger. This possibility is of particular interest, since it means that some residual reactions, typically slower (due to smaller reactant supply) than that occurring adjacent to the propellant surface, would be swept into the main chamber flow.

- (b) Besides the added complexity to any type of chamber analysis and the potential loss due to nonreacted chamber gases being ejected through the nozzle, the above phenomenon has an important bearing upon stability of the propellant-chamber configuration, whenever

$$\frac{\tau_R}{\tau_f} = \frac{\text{typical (main flow) chemical relaxation time}}{\text{characteristic chamber oscillation period}} \sim O(1) \quad (2)$$

τ_R is given by a denormalized form of the Damkohler number, based on a local mean reaction rate in the main chamber flow. For a range of frequencies up to 10 kHz, (thus, excluding ultrahigh frequencies), Eq. (2) gives the order of magnitude of τ_R for cases of interest here.

$\tau_R / \tau_f \sim O(1)$ implies that acoustic oscillation in the chamber can interact with the nonsteady heat release by chemical reactions there. The importance of coupling between pressure sensitive nonsteady heat sources and acoustic oscillations was recognized by Crocco and Cheng² and, for solid propellant configurations, by Cheng.³ This effect may be locally realized according to the so-called Rayleigh criterion:⁴ heat addition, when made at a proper point in space (i.e., in the region of a pressure antinode) and time (heat added when $p = p_{\text{max}}$, extracted when $p = p_{\text{min}}$) may have a destabilizing effect.⁵ The above criterion was recently proven to constitute a necessary condition for acoustic instability.⁶

The foregoing arguments comprise, when applicable, an additional "dimension" or degree of freedom to the coupling between acoustic processes in the chamber and the propellant. Traditionally, only the acoustic admittance of the propellant surface, $\hat{A} = -(u'/u^0)/(p'/p^0)$ or its frequency response, $\hat{F} = (m'/m^0)/p'/p^0$ were considered; now, one must account additionally for the pressure-coupled nonsteady heat release within the main chamber flow itself.

The increasing use of nitramine-based solid propellants in rocket motors motivates the present study of nonsteady reacting flows under the conditions given by Eqs. (1) and (2). Particularly, proper understanding of stability as well as quantitative assessment thereof for the chamber processes in this case is crucial, since many practical applications of these propellants exclude aluminum powder,⁷ and thereby lack mechanical means to suppress instability.

2.1.1 Physical Model

This work is an investigation of longitudinal oscillatory behavior inside an internally burning solid propellant grain with variable cross-sectional area. The frequency range is limited to the first 2 or 3 fundamental axial modes, believed to contain most of the oscillatory energy. A quasi-one-dimensional flow field is considered, with an overall second order, relatively slow exothermic chemical reaction step. The problem is treated within the framework of a fully nonlinear model, for which solutions are generated numerically. Well defined and relatively small perturbation conditions are utilized, in order to retain the ability to identify the physical mechanism involved; this also insures meaningful estimates of the numerical stability boundary and numerical spurious diffusion, so that numerical effects at all times are well understood.

The treatment of such a system within a nonlinear model has the advantage of allowing for energy exchange between the main flow and the acoustic modes, for better assessment of stability boundaries.

Within the framework of the aforementioned quasi-one-dimensional model, the following objectives are pursued in the present work:

- (a) To gain qualitative insight into the various processes that influence stability of solid propellant rocket configurations with relatively long gaseous chemical relaxation times.
- (b) On the quantitative side, to obtain for the present model stability boundaries and demonstrate the effects of geometry and thermophysical parameters on these boundaries.

The model can be described in terms of the following three elements:

(a) The main chamber flow (core flow)

For the previously defined quasi-one-dimensional system, the 4 governing equations consist of conservation laws for overall mass, momentum, energy, and a single, reference chemical species; these are written in Eulerian conservation form. Diffusion, conduction, and viscous effects were considered negligible in the axial direction; kinetic energy was included. The system is generally hyperbolic, even though a single root of the characteristic equation is repeated.

The question of dissipative terms deserves further comment here. On one hand, cases of very high axial gradients, e.g., shocks or ultrahigh frequencies, are excluded a-priori from the present framework, although the nonlinear nature of the system may admit weak solutions (those which might evolve discontinuities). On the other hand, regions where gradients are large and convection weak may be present naturally, as typical in the vicinity of an inert motor head-end closure.

To avoid this difficulty, only propellant head-end closures are considered with normal burning. Elementary steady state calculations show that Peclet numbers based on axial coordinate are in excess of $\sim O(10^4)$ at stations 0.5 port-diameters downstream of an inert head-end closure under normal rocket operating conditions. This confirms that, indeed, in the entire region considered for the core-flow processes, diffusion is negligible relative to convection.

The main flow control volume formulation allows for axial variation of the grain port. Due to the short total time of observation, time variations of geometry due to propellant consumption are extremely small and negligible in the present model.

(b) The solid phase

The solid propellant phase is represented (at each of the main chamber flow axial stations) by the nonsteady, nonlinear heat equation in a single space variable, the coordinate perpendicular to the propellant surface. Gradients and heat transfer in any of the other coordinate directions are considered negligible, as well as geometry effects upon the one-dimensionality; this is justified by the ratio (thermal layer thickness)/(typical port diameter) being much smaller than unity.

(c) The primary reaction layer

A quasi-steady, primary reaction layer separates the solid phase from the main chamber flow. The process within this layer is diffusive-reactive-convective, and considered only in the direction perpendicular to the condensed phase surface. The exothermic reactions in this layer are responsible, by heat feedback to the condensed phase, for most of the mass generation and the supply of reactants to the core flow reaction.

The layer is thin compared with typical chamber diameters, i.e., $x_R/d \ll 1$; in addition, its characteristic relaxation time is such that

$$(\delta_R/u)/\tau_f \ll 1$$

where u is a typical gas injection velocity, perpendicular to the propellant surface. Consequently, the layer is assumed to respond to both core-flow and solid phase time variations without introducing any dynamic effects; transfer inside the layer in directions other than the perpendicular to the surface are negligible. Utilizing the proper Shvab-Zeldovich coupling parameters, the formulation here reduces to a single 2-point boundary value problem, with sensible enthalpy chosen as the dependent variable. At any axial chamber location, solutions to the layer problem must match suitable

conservation conditions at both inner (chamber) and outer (propellant) interfaces, at all times. Note that the layer is nonadiabatic at both inner and outer boundaries.

2.1.2 Method of Solution

Time-dependent solution profiles to the system are obtained by forming suitable algorithms for the various elements described in the foregoing sections and solving numerically by computer.

The nonlinear partial differential system representing the main chamber flow processes is solved numerically, using a modified Rubin-Burstein⁸ explicit finite difference scheme. The original scheme was used in a similar study by Levine and Culick.⁹ The head-end and nozzle-end boundary conditions are treated by means of the local characteristic equations as suggested by Vichnevetsky,¹⁰ and used by Kuo, et al.¹¹ and Peretz, et al.¹²

The solid propellant heat equation is integrated by an Euler-explicit time marching method, with central finite differences and variable mesh size in space. This is repeated at each of the main flow axial mesh points and was found to be very efficient.

The solution to the quasi-steady primary reaction zone is generated repeatedly in an iterative scheme for each timestep in the solid and the main chamber flow. The goal is to account for correct propellant mass flux and main flow heat feedback, such that all the conservation constraints pertaining to this region are both locally and instantaneously satisfied. All the elements described above are combined in a single computer program which carries out the forward time integration for the entire system.

Solutions are being generated for a variety of propellant grain geometries: e.g., L*, port design type of axial variation of cross-sectional port area. Various extents of reaction in the main chamber flow are imposed (changing pre-exponential and activation energy) in order to find the manner by which they affect the chamber-propellant configuration response. Comparison with nonreacting chamber flows under similar conditions will be made during continuation studies.

2.1.3 Observations

To clearly identify the effects due to chemical reaction upon stability, a series of numerical experiments was designed, excluding dynamic solid phase effects. Based on the initial results, the following observations have been made.

- (a) The vicinity of the head end, which corresponds to a pressure antinode, is most sensitive to reactions in the core-flow. Considering a particular reaction (e.g., $\text{N}_2\text{O} + \text{CH}_2\text{O}$) at fixed initial pressures and frequency (about 2 kHz) there appears to be some critical port dimension [$\sim 0(1 \text{ cm})$] below which reactants can escape into the core flow and interact positively with the local acoustic field. For sufficiently large diameters (and consequently very low core flow velocities), the quasi-steady flame zone configuration is recovered. In this respect, the head-end region behavior is similar to the so-called L^* instability (where combustor residence time and characteristic chemical reaction are comparable) in a local sense, but at a much higher frequency.
- (b) The downstream end of the chamber, near the entrance to the nozzle, is the region of the second pressure antinode. Velocities here are typically larger by at least an order of magnitude than those at the head end. Due to the locally high core mass flux, high rates of heat feedback from the core to the quasi-steady layer, as well as high injected reactant concentrations, are observed; consequently, there is a decrease in the local chemical relaxation time relative to the head end. This means that a uniform imposed perturbation frequency may interact with the head-end process, as described in (a), but would be too low and therefore fail to interact with the chemical core flow process at the nozzle end. This region is also characterized by a high rate of damping of oscillations by nonlinear interaction with the mean flow. Increasing the aft-end port diameter has the same

effect as a decrease at the head end: decelerating the main flow brings about less reactant injection, less heat feedback, and higher mean pressure, leading to local increase in chemical relaxation times.

Results which include both dynamic condensed phase as well as core flow reaction effects will be developed as part of the continuation studies. Also, the trends from rocket motor firings will be interpreted in terms of the analytical results.

2.1.4 References for Section 2.1

1. BenReuven, M., Caveny, L. H., Vichnevetsky, R., and Summerfield, M., "Flame Zone and SubSurface Reaction Model for Deflagrating RDX," Proceedings of 16th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 1976, pp. 1223-1233.
2. Crocco, L., and Cheng, S. I., Rocket Instability, Butterworths, London, 1956; in particular Chapters 3 and 4, pp. 76-162.
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12. Peretz, A., Caveny, L. H., Kuo, K. K., and Summerfield, M., "The Starting Transient of Solid Propellant Rocket Motors with High Internal Gas Velocities," Aerospace and Mechanical Sciences Report No. 1100, Princeton University, Princeton, NJ, April 1973.

2.2 Unsteady Burning of Droplets*

Spray models are, at present, invariably complicated^{1**} and generally based upon knowledge of characteristics of individually burning droplets. Therefore, for practical reasons, models of single droplet combustion must be kept simple if they are to be incorporated in the more complicated spray calculations.

Because of the importance of single droplet models, our work focuses on this particular problem. The physical configuration of interest is that of an individual droplet of fuel, which we also call the liquid phase, burning in an infinite surrounding atmosphere, called the gas phase. The conditions in the far field of the gas phase can be adjusted at will.

The goal of our research was threefold. First, we wanted to understand better the domain of validity of certain classical gas-phase assumptions encountered throughout the literature on droplet combustion;^{1,2,3} those assumptions were: (1) quasi-steady gas phase, (2) flame-sheet combustion, (3) thermodynamic equilibrium at the droplet surface, and (4) same (average) molecular weight for all species. Second, based upon the insight gained in our first task, we hoped to propose a new way of studying the burning of a droplet. Finally, our third task was to apply our model to some aspects of droplet combustion.

The study of the validity of the quasi-steady gas-phase assumption was presented in Ref. 4. By carefully modeling the terms of the unsteady energy equation, we were able to predict when some of these terms were negligible. The final results were plotted in a graph which predicted the region of quasi-steady behavior of the gas phase for given kinetic and droplet characteristic times. Once these times are known, the graph indicates the region of characteristic times for external changes (at a given pressure) that does not violate the quasi-steady gas phase assumption.

*The majority of this research has been completed and is being summarized in a final report.

**References for this section are given in Section 2.2.1

The results from this work were subsequently used to develop a theory of droplet combustion which is based upon the concept of a reduced boundary condition at the droplet surface.⁵ This new theory is valid for both steady and unsteady droplet combustion. The most significant consequence of the theory is that the problem of unsteady droplet burning is reduced to the solving of a single diffusion-type nonlinear partial differential equation having one of its boundary conditions determined by an algebraic function of the quasi-steady gas-phase variables. This reduced boundary condition incorporates the entire dependence of the solution on fuel characteristics, chemical kinetics, and thermal properties of the gases. An experiment was proposed for determining this boundary condition. With the boundary condition determined experimentally, any unsteady droplet-combustion problem can be solved using realistic parameters. This boundary condition was also estimated numerically (for n-decane) by using additional assumptions.

The new theory of Ref. 5 was used in three different ways. First, it allowed us to evaluate the validity of the above-mentioned assumptions (2), (3), and (4)⁶ which are widely used in the field of droplet combustion (c.f., Refs. 7 - 14). In the study of Ref. 6, we compared a finite reaction-rate model with three flame-sheet models. These three models differed in their treatment of the evaporation from the surface and the value used for the molecular weights. The numerical computations (performed for n-decane) showed that the flame-sheet approximation is excellent at an ambient pressure of 10 atm in most of the droplet-surface temperature range. However, for surface temperatures near the boiling point or near the ambient temperature, for small droplets, or for air (as an ambient gas) with a large oxygen content, this approximation becomes unreliable. Furthermore, at lower ambient pressures (e.g., 1 atm), the assumption is shown unjustified. These conclusions are insensitive to an increase in the ambient temperature or a change in the kinetics of the finite reaction-rate model, providing this new kinetics has an imposed common solution with the previous kinetics. The thermodynamic equilibrium

assumption is shown to be valid at both $p = 10$ atm and $p = 1$ atm when the radius of the droplet is 10^{-2} cm, except for droplets having surface temperatures in the vicinity of the boiling point. For droplets with smaller radii, the approximation deteriorates even in the low temperature range. These results are not very sensitive to the ambient temperature or to the oxygen content of the ambient air. Finally, the classical flame-sheet model using the approximation of thermodynamic equilibrium at the surface and an average molecular weight was proved to be useless for practical purposes through the entire range of variation of the parameters. Of academic interest was the observation that for fixed droplet radius and ambient conditions, all theories predict very similar results at the wet bulb. A useful way of summarizing these results is to predict the validity of certain assumptions during a particular time of the droplet life. For example, it was found that during the transients associated with droplet heating (10% - 20% of the droplet lifetime) the only adequate assumption is that of thermodynamic equilibrium at the surface (for droplets of radius larger than 10^{-3} cm). In the temperature range usually associated with unsteady burning of droplets (surface temperature smaller than wet-bulb temperature, but not near the ambient) the flame-sheet assumption becomes inappropriate as the radius of the droplet or the ambient pressure decreases, or as the oxygen content of the ambient air increases. Considerable discrepancies between Models 1 - 3 were found in the vicinity of the boiling point.

The new theory of droplet burning⁵ was also used to study the possibility of extinguishing droplets by a depressurization of the gas phase.¹⁵ The investigation was motivated by the desirability of optimizing between the power output and the NO pollution in many power systems using fuel sprays.⁸ Our work demonstrated the possibility of extinction by depressurization for both regressing and non-regressing droplets. Extinction boundaries, numerically evaluated (for n-decane) as functions of different parameters showed that: (1) regressing droplets extinguish faster than non-regressing droplets at the same depressurization rate, (2) the extinction pressure is a decreasing function of the depressurization

rate, (3) the extinction boundary is a weak function of the initial droplet-temperature profile for regressing droplets, whereas the opposite is true for constant-size droplets, and (4) the extinction boundary is an increasing function of the initial pressure for both types of droplets but the extinction pressure is a non-monotonic function of the same variable for constant-size droplets and an increasing function for regressing droplets. Smaller activation energies hinder extinction, whereas smaller Arrhenius law pre-exponential constants do the opposite. The mass diffusivity of the liquid phase has almost no influence on the extinction boundary.

Finally, using the concept of Ref. 6 for droplet evaporation (instead of burning), we analyzed the influence of chemical kinetics upon thermal ignition of droplets.¹⁶ Since activation energies can be experimentally predicted only within a few kilocalories and the pre-exponential constants (in the Arrhenius law) within an order of magnitude, all ignition criteria using fixed kinetics during the preignition period^{17,18} may suffer large uncertainties in the prediction of the ignition-delay time. Our reasoning was that the mathematical model should reflect the change in kinetics due to various decomposition reactions in the gas phase successively becoming dominant during the preignition period. Since the kinetics of these intermediate reactions are unknown, we made the kinetics function of the maximum possible temperature in the gas phase. Two functions having each two free parameters were used to obtain temperature-varying kinetics; one function was exponential, the other linear. The two free parameters were determined by requiring that at the ambient temperature the kinetics correspond to typical induction kinetics, and that at a typical flame-sheet temperature for combustion the kinetics are those of a well-developed flame. By using the ignition criterion of Law,¹¹ we showed that when the kinetics are constant during the preignition period the ignition-delay time is a strong function of the kinetics. However, when a variable kinetics is used, the predicted ignition times are very close together, independently of

the initial induction kinetics, or of the chosen temperature variation. The numerical computations, performed (for n-decane) for conditions characteristic of the injection time in Diesel engines, showed that whereas for a droplet with an initial radius of 10^{-2} cm the ignition-delay time uncertainty obtained with various constant inductive kinetics is about a sixth of the total combustion time in a Diesel engine at 1200 rpm, this uncertainty becomes a thirtieth of the total combustion time when variable kinetics are used. For a droplet with an initial radius of 0.5×10^{-2} cm these numbers are respectively a fifth and zero. Although these numbers will change both with the assumed final kinetics and the value of the maximum gas phase temperature at this final kinetics, the qualitative trends should remain. Thus, the usual experimental chemical kinetics uncertainties are acceptable providing that (1) the maximum temperature (in the gas field) that is associated with a given kinetics is known, and (2) a variable kinetics (depending upon this maximum gas field temperature) are used to compute the ignition-delay time.

2.2.1 References for Section 2.2

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3. Williams, A., "Combustion of Droplets and Liquid Fuels: A Review," Combustion and Flame, Vol. 21, (1973), pp. 1-31.
- *4. Bellan, J. and Summerfield, M., "Quasi-Steady Gas Phase Assumption for a Burning Droplet," AIAA Journal, Vol. 14, (1976), pp. 973-975.
- *5. Bellan, J. and Summerfield, M., "Model for Studying Unsteady Droplet Combustion," AIAA Journal, Vol. 15, (1977), pp. 234-242.
- *6. Bellan, J. and Summerfield, M., "Theoretical Examination of Assumptions Commonly Used for the Gas Phase Surrounding a Burning Droplet," submitted to Combustion and Flame.

*Abstract included in Section 3.

7. Polymeropoulos, C. E. and Peskin, R. L., "Ignition and Extinction of Liquid Fuel Drops - Numerical Computations," Combustion and Flame, Vol. 13, pp. 166-172.
8. Bracco, F., "Nitric Oxide Formation in Droplet Diffusion Flames," Proceedings of the 14th International Symposium on Combustion, (1972), pp. 831-841.
9. Canada, G. S. and Faeth, G. M., "Fuel Droplet Burning Rates at High Pressures," Proceedings of the 14th International Symposium on Combustion, (1972), pp. 1345-1354.
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11. Law, C. K., "Asymptotic Theory for Ignition and Extinction in Droplet Burning," Combustion and Flame, Vol. 24, pp. 89-98.
12. Law, C. K., "Unsteady Droplet Combustion with Droplet Heating," Combustion and Flame, Vol. 26, pp. 17-22.
13. Law, C. K., "Multi-Component Droplet Combustion with Rapid Internal Mixing," Combustion and Flame, Vol. 26, pp. 219-233.
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- *15. Bellan, J. and Summerfield, M., "A Theoretical Study of Droplet Extinction by Depressurization," Presented at Spring Technical Meeting of Combustion Institute, March 1977.
16. Bellan, J. and Summerfield, M., "A theoretical Model Using Temperature-Dependent Kinetics to Predict Droplet Thermal-Ignition Lag," to be submitted to AIAA Journal.
17. Faeth, G. M. and Olson, D. R., "The Ignition of Hydrocarbon Fuel Droplets in Air," SAE Transactions, Vol. 77 (1968), Sec. 3, pp. 1793-1802.
18. Law, C. K., "Analysis of Thermal Ignition Lag in Fuel Droplet Combustion," Paper preprinted for the Central States Meeting of the Combustion Institute, Cleveland, Ohio, 1977.

*Abstract included in Section 3.

3.0 RECENT PUBLICATIONS UNDER ONR FUNDING

Abstracts of these publications are given in Section 3.4.

3.1 Manuscript Submission During Reporting Period

1. BenReuven, M., Caveny, L. H., Vichnevetsky, R., and Summerfield, M., "Unsteady Reacting Flows in Solid Rocket Chambers," AIAA Preprint 78-948, accepted for presentation at the AIAA 14th Propulsion Conference, July 25-27, 1978.
2. Bellan, J. and Summerfield, M., "A Theoretical Study of Droplet Extinction by Depressurization," Presented at the 1977 Spring Technical Meeting of the Combustion Institute, Central States Section, March 1977, accepted by Combustion and Flame for publication.
3. Bellan, J. and Summerfield, M., "Theoretical Examination of Assumptions Commonly Used for the Gas Phase Surrounding a Burning Droplet," accepted by Combustion and Flame for publication.
4. Bellan, J. and Summerfield, M., "Comparison of Four Models Describing Combustion of Droplets," preprinted for Technical Meeting of Combustion Institute/Eastern Section, November 1976, submitted to Combustion and Flame for publication.

3.2 Publications That Have Appeared During Reporting Period

1. BenReuven, M., Caveny, L. H., Vichnevetsky, R., and Summerfield, M., "Flame Zone and Sub-Surface Reaction Model for Deflagrating RDX," Proceedings of 16th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 1976, pp. 1223-1233.
2. Bellan, J. and Summerfield, M., "A Model for Studying Unsteady Droplet Combustion," AIAA Journal, Vol. 15, No. 2, February 1977, pp. 234-242.

3.3 Recent Publications Under ONR Funding Prior to this Reporting Period

1. Alkidas, A. C., Morris, S. O., Caveny, L. H., and Summerfield, M., "An Experimental Study of Pressure Wave Propagation in Granular Propellants," AIAA Journal, June 1976, pp. 789-792.
2. Bellan, J. and Summerfield, M., "On Quasi-Steady Assumptions for a Burning Droplet," AIAA Journal, July 1976, pp. 973-975.

3.4 Abstracts of Publications

On the following pages are the abstracts of the publications listed below.

1. "Unsteady Reacting Flows in Solid Rocket Chambers, M. BenReuven, L. H. Caveny, R. Vichnevetsky and M. Summerfield, AIAA Preprint 78-948, accepted for presentation at the AIAA 14th Propulsion Conference, July 25-27, 1978.
2. "A Theoretical Study of Droplet Extinction by Depressurization," J. Bellan and M. Summerfield, Spring Technical Meeting of the Central States Section/The Combustion Institute, March 1977, also accepted for publication in Combustion and Flame.
3. "Theoretical Examination of Assumptions Commonly Used for the Gas Phase Surrounding a Burning Droplet," J. Bellan and M. Summerfield, accepted by Combustion and Flame for publication.
4. "Comparison of Four Models Describing Combustion of Droplets," J. Bellan and M. Summerfield, Presented at 1976 Technical Meeting of the Eastern Section, The Combustion Institute, November 1976, submitted to Combustion and Flame for publication.
5. "Flame Zone and Sub-Surface Reaction Model for Deflagrating RDX," M. BenReuven, L. H. Caveny, R. J. Vichnevetsky, and M. Summerfield, Proceedings of 16th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 1976, pp. 1223-1233.
6. "A Model for Studying Unsteady Droplet Combustion," J. Bellan and M. Summerfield, AIAA Journal, Vol. 15, No. 2, February 1977, pp. 234-242.

7. "An Experimental Study of Pressure Wave Propagation in Granular Propellant Beds," A. C. Alkidas, S. O. Morris, L. H. Caveny and M. Summerfield, AIAA Journal, Vol. 14, No. 6, June 1976, pp. 789-792.
8. "On the Quasi-Steady Assumptions for a Burning Droplet," J. Bellan and M. Summerfield, AIAA Journal, Vol. 14, No. 7, July 1976, pp. 973-975.

UNSTEADY REACTING FLOWS IN SOLID ROCKET CHAMBERS

M. BenReuven, L. H. Caveny, R. Vichnevetsky and M. Summerfield

AIAA Preprint 79-948, accepted for presentation at AIAA 14th Propulsion Meeting, July 25-27, 1978.

The unsteady responses of high temperature gases in solid propellant rocket chambers are usually analyzed by assuming a collapsed, quasi-steady chemical reaction zone, adjacent to the propellant surface. Clearly, the quasi-steady gaseous flame zone assumption holds for a large class of propellants whose chemical relaxation times are sufficiently short. However, that assumption does not apply for propellants which exhibit relatively long secondary reaction zones, e.g., nitramine composite propellants. This work is an investigation of longitudinal oscillatory behavior of the chamber flow coupled to the dynamic burning responses of the propellant. A quasi-one-dimensional flow field is considered, with an overall second order, relatively slow exothermic chemical reaction step. The vicinity of the head end is most sensitive to reactions in the core-flow. Considering a particular reaction (e.g., $\text{N}_2\text{O} + \text{CH}_2\text{O}$) at fixed initial pressures and frequency (about 2 kHz) there appears to be some critical port dimension [$\sim 0(1 \text{ cm})$] below which reactants can escape into the core flow and interact positively with the local acoustic field. For sufficiently large diameters (and consequently very low core flow velocities), the quasi-steady flame zone configuration is recovered. In the downstream end of the chamber, due to the locally high core mass flux, rates of heat feedback from the core to the quasi-steady layer are high. Thus, high injected reactant concentrations are observed. Consequently, there is a decrease in the local chemical relaxation time relative to the head end. This means that a uniform imposed perturbation frequency may interact with the head-end process but would be too low and therefore fail to interact with the chemical core flow process at the nozzle end. This region is also characterized by a high rate of damping of oscillations by nonlinear interaction with the mean flow.

Based on work performed under Contract N00014-75-C-0705 issued by the Office of Naval Research and supplemented by the U.S. Army Ballistic Research Laboratory.

A THEORETICAL STUDY OF DROPLET EXTINCTION BY DEPRESSURIZATION

Josette Bellan and Martin Summerfield

Spring Technical Meeting of the Central States Section/The Combustion Institute, March 1977, also accepted for publication in Combustion and Flame.

Depressurization-induced extinction of droplets is demonstrated using a previously presented quasi-steady gas-phase model. It is shown, in particular, that depressurization of the gas phase causes extinction for both regressing and non-regressing droplets. Extinction boundaries, numerically evaluated as functions of different parameters show that: (1) regressing droplets extinguish faster than non-regressing droplets at the same depressurization rate, (2) the extinction pressure is a decreasing function of the depressurization rate, (3) the extinction boundary is a weak function of the initial droplet-temperature profile for regressing droplets, whereas the opposite is true for constant-size droplets, (4) the extinction boundary is an increasing function of the initial pressure for both types of droplets, but the extinction pressure is a nonmonotonic function of the same variable for constant-size droplets and an increasing function for regressing droplets. Smaller activation energies hinder extinction, whereas smaller Arrhenius-law pre-exponential constants do the opposite. The mass diffusivity of the liquid phase has almost no influence on the extinction boundary.

Work performed under Contract N00014-75-C-0705 sponsored by the Office of Naval Research.

THEORETICAL EXAMINATION OF ASSUMPTIONS COMMONLY USED FOR THE GAS
PHASE SURROUNDING A BURNING DROPLET

J. Bellan and M. Summerfield

Accepted by Combustion and Flame for publication.

A finite reaction rate model is compared to three commonly used flame-sheet models. These three models differ in their treatment of the evaporation from the surface and the value used for the molecular weights. All four models are valid for both steady and unsteady burning of droplets. Further, they account for variations of droplet radii and allow for differences in ambient conditions. Numerical results (obtained for n-decane) show that if the radius of the droplet is 10^{-2} cm the thin flame approximation is excellent at 10 atm if the droplet surface temperature is not close to either the boiling point or the ambient temperature. However, this approximation is unacceptable at 1 atm. Among the three flame-sheet models, the one using non-equilibrium evaporation at the surface and individual molecular weights best approximates the finite reaction rate theory. However, this agreement breaks down for smaller droplets with lower surface temperatures, or for air with a larger oxygen content. These conclusions are independent of the chosen kinetics. The Clausius-Clapeyron approximation is shown to be excellent away from the boiling point for $R = 10^{-2}$ cm. However, as the droplet surface temperature approaches the boiling point, or the droplet radius decreases, this assumption leads to considerable errors in the evaporation rate and also distortion of the thermal layer. Even larger errors are obtained when an average molecular weight is used. Here, large underestimates of the evaporation rate and great distortions of the thermal layer of the droplet are obtained. In spite of these errors, all four models agree at wet-bulb conditions.

Based on work performed under Contract N00014-75-C-0705 issued by the Office of Naval Research.

"COMPARISON OF FOUR MODELS DESCRIBING COMBUSTION OF DROPLETS"

Josette Bellan and Martin Summerfield

Presented at the 1976 Technical Meeting of the
Eastern Section, The Combustion Institute, November 1976

The comparison is made between a formulation using a finite reaction rate and three other formulations based upon the flame-sheet approximation. The difference among these latter models consists in the treatment of the evaporation from the surface and also of the molecular weights. The theory is valid for steady or unsteady burning of droplets. Numerical results for decane show that the thin flame approximation is excellent at 10 atm but unacceptable at 1 atm. Among the flame-sheet models, the one using nonequilibrium evaporation and individual molecular weights approximates best the finite reaction rate theory. This good agreement breaks down in more-oxidant-than-air ambient atmospheres. The Clausius-Clapeyron approximation is shown to be excellent at 10 atm and still good at 1 atm. When averaging the molecular weights large underestimates of the evaporation rate are obtained. The thermal layer of the droplet is also greatly misestimated.

Based on work performed under sponsorship of the Office
of Naval Research under Contract N00014-75-C-0705.

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the Engineering Societies Library, New York, N.Y.

"FLAME ZONE AND SUB-SURFACE REACTION MODEL FOR DEFLAGRATING RDX"

M. BenReuven, L. H. Caveny, R. J. Vichnevetsky, and M. Summerfield

Proceedings of 16th Symposium (International) on Combustion,
The Combustion Institute, Pittsburgh, PA, 1976, pp. 1223-1233.

A study of 1,3,5 Trinitro Hexahydro 1,3,5, Triazine, RDX, burning as a monopropellant was undertaken to obtain a better understanding of the important chemical steps that control heat feedback to the condensed phase, to determine the contributions of the liquid layer, and to provide a means of evaluating theories for modifying the burning rate of nitramines. The following chemical mechanism is proposed: first, partial decomposition of RDX molecule in the liquid phase; second, following vaporization, gas phase decomposition of RDX; third, oxidation of formaldehyde by NO_2 . The flame structure and liquid layer reactions of deflagrating RDX were expressed in terms of the energy, continuity, and species equations corresponding to RDX decomposing in liquid and gaseous phases and the $\text{NO}_2/\text{CH}_2\text{O}$ reactions adjacent to the surface. In addition to the temperature profile and burning rate, the numerical solution provides the details of the interactions at the liquid/gas interface and the concentration profiles for the nine most prominent species. Using published kinetic data, the calculated results reveal that even though the liquid layer becomes thinner with increasing pressure, the increase in surface temperature causes its heat feedback contribution to increase. The pressure sensitivity of burning rate between 0.7 and 0.8 is interpreted in terms of the relative contributions of gas phase and liquid layer RDX decomposition and the oxidation of CH_2O . In particular, as pressure increases, the contribution from liquid layer reactions and the second order, $\text{NO}_2/\text{CH}_2\text{O}$ reaction become more prominent.

Based on work performed under Contract N00014-75-C-0705
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A MODEL FOR STUDYING UNSTEADY DROPLET COMBUSTION

Josette Bellan and Martin Summerfield

AIAA Journal, Vol. 15, No. 2, February 1977, pp. 234-242.

The concept of a reduced boundary condition at the surface of a droplet is used to develop a new theory of unsteady droplet burning. This theory utilizes a quasi-steady gas phase assumption which has been shown to be realistic for a wide range of droplet sizes at low pressures. The most significant consequence of the theory is that the problem of unsteady droplet burning is reduced to the solving of a single diffusion-type nonlinear partial differential equation having one of its boundary conditions determined by an algebraic function of the quasi-steady gas phase variables. This reduced boundary condition incorporates the entire dependence of the solution on fuel characteristics, chemical kinetics and thermal properties of the gases. An experiment is proposed for determining this boundary condition so that the nonsteady droplet combustion problem can be solved for a realistic situation. By using additional assumptions, a numerical estimate of the boundary condition has been made.

Based on work performed under contract N00014-75-C-0705 sponsored by the Office of Naval Research.

Above cited article supersedes AIAA Paper 76-614, July 1975.

"AN EXPERIMENTAL STUDY OF PRESSURE WAVE PROPAGATION IN GRANULAR PROPELLANT BEDS."

A. C. Alkidas, S. O. Morris, L. H. Caveny and M. Summerfield

AIAA Journal, Vol. 14, No. 6, June 1976, pp. 789-792.

The ignition transients and penetrative burning characteristics of confined granular propellant beds in a cylindrical tube (loading densities up to 1.03 g/cm^3 and pressures up to 4000 bar) were investigated to test the 1-D pressure-wave propagation profiles predicted by the 1971 Kuo-Vichnevetsky-Summerfield analytical model. Thus, it was found that following the initial pressure rise along the bed, the position of peak pressure occurs within the bed and progresses downstream at an accelerating rate. The ignition time of the granular bed increases sharply with decreasing loading density. However, the pressurization time depends primarily on the diameter and burning rate of the granules that make up the bed. Wall friction acting on the unburned propellant along the tube attenuates downstream transmission of solid phase pressure generated by the upstream burning processes. This work has applications to the internal ballistics of guns, deflagration to detonation transition, and fast burning rocket charges.

Based on work performed under sponsorship of the Power Branch of the Office of Naval Research under contract N00014-67-A-0151-0023.

Journal article supercedes AIAA Paper No. 75-242, January 1975. Accession No. A75-20292 for AIAA Paper No. 75-242. Available from AIAA.

"ON THE QUASI-STEADY ASSUMPTIONS FOR A BURNING DROPLET."

Josette Bellan and Martin Summerfield

AIAA Journal, Vol. 14, No. 7, July 1976, pp. 973-975.

A large number of results obtained in the field of droplet combustion are based upon the assumption that the gas field behaves in a quasi-steady manner. However, this assumption is introduced usually without adequate justification. Therefore, it is felt here that the discussion on the possibility of realistically making the quasi-steady assumption for the gas phase deserves particular attention. It was shown that for droplets in the range encountered in Diesel engines or rockets, there is a domain in the plane (τ_p, p) (τ_p is a characteristic time and p is a pressure) where the quasi-steady assumption is valid for typical pressures developed in the above combustion systems. As the droplet size decreases, the domain is shown to be larger.

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produce flame zones which extend well into the main chamber flow field. An analytical model is being developed that considers the effects of chemical reactions (i.e., extended flame zones) in the main chamber flow on the acoustic response of solid rocket motors.

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PREFACE

This research was carried out under Contract N00014-75-C-0705 from the Power Branch, Office of Naval Research. Dr. Richard S. Miller, of the Power Branch, is the Project Monitor. The U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, provided partial support for this research. Mr. C. W. Nelson is providing technical liaison with the Army.

The text of this report summarizes work that is in progress; by the end of 1978 more recent versions of the work will be available.

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